Discrete scale invariance and Efimov bound states in Weyl systems with coexistence of electron and hole carriers

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arXiv:1704.00995

Supported by



- 1. Experimental results and general background
- Log-periodic magneto-resistance in ultra-quantum ZrTe5
- Brief introduction to discrete scale invariance and Efimov physics
- 2. Possible Fermionic Efimov bound states
- Three-body Schrödinger case with resonant scattering
- Two-body Weyl Hamiltonian with Coulomb attraction
- Influence of magnetic field and comparison to experiments
- 3. Conclusions

Log-B periodic magneto-resistance oscillation in ZrTe₅



Log-B periodic MR oscillations from 0.2T to 55T.

Discrete Scale Invariance in ZrTe₅ beyond the quantum limit



Discrete Scale Invariance in ultra-quantum in ZrTe₅ with coexistence of heavy electron (low mobility) and light hole (high mobility). ⁵

Discrete scale invariance



Efimov spectrum

Mandelbrot set



D. Sornette, Physics Reports 297 239 (1998). E. Braaten, H.-W. Hammer, Physics Reports 428 259 (2006).

Bosonic Efimov trimers (resonant scattering)

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PHYSICS LETTERS

21 December 1970

ENERGY LEVELS ARISING FROM RESONANT TWO-BODY FORCES IN A THREE-BODY SYSTEM

> V. EFIMOV A.F. Ioffe Physico-Technical Institute, Leningrad, USSR

> > Received 20 October 1970

When 2 bosons interact with infinite scattering length *a*, 3 bosons always form a geometric series of bound states.



 $e^{\pi/s_0} \approx 22.7$ with $s_0 \approx 1.006$

Discrete Scale Invariance

Resonant scattering (obtained by Feshbach resonance)



Efimov trimer of identical bosons (near resonance)





$$E_{\mathrm{T}}^{(n)} \longrightarrow (e^{-2\pi/s_0})^{n-n_*} \frac{\hbar^2 \kappa_*^2}{m} \quad a = \pm \infty.$$

- 1. 1/R² attraction is a requisite.
- 2. Energy spectrum also show Discrete Scale Invariance.





E. Braaten, H.-W. Hammer, Physics Reports 428 259 (2006).

Efimov trimer of identical bosons (experimental realization)



Rudolf Grimm, Nature 440, 315 (2006); PRL 112, 190401 (2014); Reinhard Dörner, Science 348, 551 (2015); Matthias Weidemüller, PRL 112, 250404 (2014); Cheng Chin, PRL 113, 240402 (2014).

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Efimov attraction from Born-Oppenheimer approximation



Trimer wave-function

$$\psi_T(R,r) = F_{2e}(R)\phi_h(r,R)$$

Schrödinger equation for hole wave-function $-\hbar^2/2M_h \nabla_r^2 \phi_h(r, R) = \varepsilon_h \phi_h(r, R)$

Hole wave-function: $\phi_h(r, R) = \frac{\exp[-k_h|r - R/2|]}{|r - R/2|} + \frac{\exp[-k_h|r + R/2|]}{|r + R/2|}$

Decay wave-number:
$$k_h = \frac{1}{\hbar} \sqrt{-2M_h \varepsilon_h}$$

Bethe-Peierls boundary condition: $\frac{\partial}{\partial r}(r\phi_h)_{r\to 0} \to -\frac{1}{a} \to k_h R - e^{-k_h R} = \frac{R}{a}$

 $k_h R = \Omega \approx 0.567$ Solution of $\Omega = e^{-\Omega}$ when scattering length $a \to \pm \infty$

Energy of hole:

$$\varepsilon_h(R) \sim -\frac{\hbar^2}{2M_h} \frac{\Omega^2}{R^2}$$

Efimov attraction from Born-Oppenheimer approximation

Schrödinger equation for two electrons (center of mass):

$$\left[-\frac{\hbar^2}{M_e}\nabla_R^2 + \varepsilon_h(R)\right]F_{2e}(R) = E_T \cdot F_{2e}(R)$$

Wave-function for two electrons (center of mass):

$$F_{2e}(R) = R^{-1}f(R)Y_{LM}(\theta)$$

Differential equation for radical part:

$$\left(-\frac{d^2}{dR^2} + V(R) - \frac{M_e E_T}{\hbar^2}\right) f(R) = 0$$

Efimov attraction:

$$V(R) = \frac{L(L+1)}{R^2} - \frac{M_e \Omega^2}{2M_h R^2} = \frac{-s_0^2 - 1/4}{R^2}$$

Definition: (real *s*⁰ guarantee a solution)

$$|s_0|^2 = \frac{M_e}{2M_h} \Omega^2 - L(L+1) - \frac{1}{4}$$

Identical fermions:L = 1real s_0 contraint: $\frac{M_e}{M_h} > 13.6$ This constraint can
be matched in solid
state systems.

Efimov Trimers from the Born-Oppenheimer approximation

Differential equation for radical part (with real positive *s*₀):

$$\left[-\frac{d^2}{dR^2} - \frac{s_0^2 + 1/4}{R^2} - \frac{M_e E_T}{\hbar^2}\right] f(R) = 0 \quad \text{[Landau \& Lifshitz QM]}$$

Definitions and differential equation for auxiliary function:

$$E_T = -\frac{\hbar^2 k_T^2}{M_e} \qquad f(R) = R^{\frac{1}{2}} g(R) \qquad \tilde{R} = k_T R$$
$$g''(\tilde{R}) + \frac{1}{\tilde{R}} g'(\tilde{R}) + \left(-1 + \frac{s_0^2}{\tilde{R}^2}\right) g(\tilde{R}) = 0$$

E= E_T Solution: $f(R) = R^{\frac{1}{2}}K_{is_0}(k_T R)$ $f(R) \sim R^{\frac{1}{2}}\sin[s_0\ln(k_T R) + \alpha]$

E \approx **o Solution:** $f_1(R) \approx AR^{\frac{1}{2}} \sin[s_0 \ln k_* R + \alpha]$

Match the wave-function at boundary.

Continuous condition of $R \frac{f'(R)}{f(R)}$ at **boundary**.

Discrete Scale Invariance

$$k_{T,n} = \left(e^{-\pi/s_0}\right)^{n-n_0} e^{-\alpha/s_0} k_*$$
$$E_{B,n} = \left(e^{-2\pi/s_0}\right)^{n-n_0} \frac{\hbar^2 \tilde{k}_*^2}{M_e}$$
$$\langle R_n^2 \rangle \propto k_{T,n}^{-2} \quad \frac{R_{n+1}}{R_n} = e^{\pi/s_0}$$
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$$H = \frac{1}{2M_h} \left(-i\hbar \vec{\nabla}_1 - \frac{e}{c} \vec{A}_1 \right)^2 + \frac{1}{2M_e} \left(-i\hbar \vec{\nabla}_2 + \frac{e}{c} \vec{A}_2 \right)^2 + \frac{1}{2M_e} \left(-i\hbar \vec{\nabla}_3 + \frac{e}{c} \vec{A}_3 \right)^2$$

Under small magnetic field, the binding energy of Efimov bound states $|E_T|$ is much larger than the Landau level spacing.

The magnetic field can be treated as perturbation, and the system still **possesses** approximate hyper-spherical symmetry.

In hyper-spherical coordinates: *harmonic oscillator potential*

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$$\begin{pmatrix} -\nabla_{\vec{r}_{ij}}^2 - \nabla_{\vec{\rho}_{ij,k}}^2 + \frac{M_e^2 \omega_B^2 R^2}{8\hbar^2} + \frac{M_e \omega_B}{2\hbar^2} \hat{L}_{ij,k}^z - \frac{M_e E_T}{\hbar^2} \end{pmatrix} \Psi = 0$$

hyper-spherical $-\nabla_{\vec{r}_{ij}}^2 - \nabla_{\vec{\rho}_{ij,k}}^2 = \frac{\hat{L}_{ij}^2}{\hbar^2 R^2 \sin^2 \vartheta_k} + \frac{\hat{L}_{ij,k}^2}{\hbar^2 R^2 \cos^2 \vartheta_k}$
operators: $+R^{-\frac{5}{2}} \left[-\frac{\partial^2}{\partial R^2} + \frac{15}{4R^2} \right] R^{\frac{5}{2}} + \frac{1}{R^2 \sin 2\vartheta_k} \left[-\frac{\partial^2}{\partial \vartheta_k^2} - 4 \right] \sin 2\vartheta_k$

Influence of magnetic field on Efimov trimers: small B

The Faddeev decomposition:

$$\Psi = \varphi^{(1)}(\vec{r}_{23}, \vec{\rho}_{23,1}) + \varphi^{(2)}(\vec{r}_{13}, \vec{\rho}_{13,2}) - \varphi^{(2)}(\vec{r}_{12}, \vec{\rho}_{12,3})$$

The Faddeev equation:

$$\left(-\nabla_{\vec{r}}^2 - \nabla_{\vec{\rho}}^2 + \frac{M_e^2 \omega_B^2 R^2}{8\hbar^2} + \frac{M_e \omega_B}{2\hbar^2} \hat{L}_{ij,k}^z - \frac{M_e E_T}{\hbar^2}\right) \varphi^{(i)}(\vec{r},\vec{\rho}) = 0$$

Solution ansatz:

$$\varphi^{(i)}(\vec{r},\vec{\rho}) = \frac{\varphi_0^{(i)}(R,\vartheta,\hat{\rho})}{R^{5/2}\sin 2\vartheta} = \frac{1}{R^{5/2}\sin 2\vartheta} \sum_{n,l,m} f_{n,l}^{(i)}(R) \phi_{n,l}^{(i)}(\vartheta;R) Y_{lm}(\hat{\rho})$$

The hyper-angle equation (l = 1):

$$\left(-\frac{\partial^2}{\partial\vartheta^2} + \frac{l(l+1)}{\cos^2\vartheta}\right)\phi_{n,l}^{(i)}(\vartheta;R) = s_{n,l}^2\phi_{n,l}^{(i)}(\vartheta;R)$$

Bethe-Peierls boundary condition: $\frac{1}{r\Psi}\frac{\partial}{\partial r}(r\Psi) \xrightarrow[r \to 0]{} - \frac{1}{a}$

$$-\frac{1}{a}$$
 $\sin \gamma = \frac{M_e}{M_h + M_e}$

Eigenvalues:

$$\frac{1-s_n^2}{s_n} \tan\left(s_n \frac{\pi}{2}\right) - \frac{2\cos(\gamma s_n)}{\sin(2\gamma)\cos(s_n \frac{\pi}{2})} + \frac{\sin(\gamma s_n)/s_n}{\sin^2\gamma\cos(s_n \frac{\pi}{2})} = 0$$

The above secular equation have imaginary solution $s_n = is_0$ if $\gamma > 1.199$, corresponding to $M_e/M_h > 13.6$.



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Influence of magnetic field: approximate discrete scale invariance

The hyper-radial equation:

$$\left(-\frac{d^2}{dR^2} - \frac{s_0^2 + 1/4}{R^2} + \frac{R^2}{4l_B^4} + \frac{1}{2l_B^2}\right) f_n(R) = \frac{M_E E_T}{\hbar^2} f_n(R)$$

Attractive potential condition:

$$-\frac{s_0^2 + 1/4}{R^2} + \frac{R^2}{4l_B^4} + \frac{1}{2l_B^2} < 0 \qquad \blacksquare \qquad R < R_c \equiv \sqrt{2s_0} l_B$$

WKB solution of Efimov trimers:

$$\oint pdr \approx 2\hbar \int_{R_0}^{R_n} \frac{s_0}{R} \sqrt{1 - \frac{R^2}{2s_0 l_B^2}} dR = 2\pi n\hbar$$

Approximate discrete scale invariance for $R_n < R_c$:

$$\ln \frac{R_n}{R_{n-1}} = \frac{\pi}{s_0} + \frac{R_n^2}{4s_0^2 l_{B_n}^2} - \frac{R_{n-1}^2}{4s_0^2 l_{B_{n-1}}^2} \in \left(\frac{\pi}{s_0} - \frac{1}{2s_0}, \frac{\pi}{s_0} + \frac{1}{2s_0}\right)$$
$$\ln \frac{B_{n+1}}{B_n} \in \left(-\frac{2\pi}{s_0} - \frac{1}{s_0}, -\frac{2\pi}{s_0} + \frac{1}{s_0}\right)$$

Problem, comparison and solution \rightarrow from 3-body to 2-body

- 1. How to obtain the resonant scattering condition $a \rightarrow \pm \infty$ with large magnetic field?
- Not clear. Thus, the prerequisite for Efimov trimers is not met.

2. In the large magnetic field limit, the system become quasi-1D with cylindrical symmetry. No Efimov trimers in 1D.

3. ZrTe₅ is identified as Dirac semimetal by ARPES [Nature Physics 12, 550 (2016)], what's the influence of Dirac physics?

Efimov equation: $\begin{bmatrix} -\frac{d^2}{dR^2} - \frac{s_0^2 + 1/4}{R^2} - \frac{M_e E_T}{\hbar^2} \end{bmatrix} f(R) = 0$ Scale Invariant Dirac equation: $\begin{bmatrix} m & \hbar v_F \vec{\sigma} \cdot \vec{k} \\ \hbar v_F \vec{\sigma} \cdot \vec{k} & -m \end{bmatrix} \Psi = \begin{bmatrix} E - V(\vec{R}) \end{bmatrix} \Psi$

Scale invariance is obtained, if m = 0 and $V(\vec{R}) \propto R^{-1}$.

Weyl semimetal with Coulomb attraction.

Dirac particle with Coulomb attraction

Dirac-Kepler problem at large Z, atomic collapse 3D W. Greiner, B. Muller & J. Rafelski, QED of Strong Fields (Springer, 1985). Y. B. Zeldovich and V. S. Popov, Usp. Fiz. Nauk 105, 403 (1971).



Atomic collapse in graphene 2D

A. V. Shytov, M. I. Katsnelson, and L. S. Levitov, PRL 99, 236801 (2007).

A. V. Shytov, M. I. Katsnelson, and L. S. Levitov, PRL 99, 246802 (2007).

V. M. Pereira, J. Nilsson, and A. H. Castro Neto, PRL 99, 166802 (2007).

Quasi-bound states in the supercritical regime of graphene.

3D Weyl particle + Coulomb attraction + magnetic field

$$\begin{bmatrix} 0 & \hbar v_F \left(\vec{\sigma} \cdot \vec{k} + \frac{e}{\hbar c} \vec{\sigma} \cdot \vec{A} \right) \\ \hbar v_F \left(\vec{\sigma} \cdot \vec{k} + \frac{e}{\hbar c} \vec{\sigma} \cdot \vec{A} \right) & 0 \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix} = \begin{bmatrix} E - V(R) \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix}$$

Under small magnetic field, the Coulomb attraction $|E_T|$ is much larger than the Landau level spacing.

Expanding in spinor spherical harmonic function:

$$\begin{bmatrix} \Psi_1\left(\vec{R}\right)\\ \Psi_2\left(\vec{R}\right) \end{bmatrix} = \begin{bmatrix} Y_{\lambda-1}^{\lambda-\frac{1}{2},m}(\theta,\varphi) \, u_1(R)/R\\ Y_{\lambda-1}^{\lambda-\frac{1}{2},m}(\theta,\varphi) \, u_2(R)/R \end{bmatrix}$$

Radial equation:

$$\frac{d}{dR} \begin{bmatrix} u_1(R) \\ u_2(R) \end{bmatrix} = \begin{bmatrix} \frac{\lambda}{R} + \frac{R}{2l_B^2} & \frac{E}{\hbar v_F} + \frac{Z\alpha}{R} \\ -\left(\frac{E}{\hbar v_F} + \frac{Z\alpha}{R}\right) & -\left(\frac{\lambda}{R} + \frac{R}{2l_B^2}\right) \end{bmatrix} \begin{bmatrix} u_1(R) \\ u_2(R) \end{bmatrix}$$

Approximate discrete scale invariance

Radial equation (i=1,2) : $\frac{d^2}{dR^2}u_i(R) = \left(\frac{\lambda}{R} + \frac{R}{2l_p^2}\right)^2 u_i(R) - \left(\frac{E}{\hbar v_E} + \frac{Z\alpha}{R}\right)^2 u_i(R)$ Magnetic field B=0: $p_R \approx \frac{\hbar s_0}{D} \qquad s_0 \equiv \sqrt{(Z\alpha)^2 - \lambda^2}$ WKB solution: $p_R \approx \frac{\hbar}{R} \left| (Z\alpha)^2 - \left(\lambda + \frac{R^2}{2l_B^2}\right)^2 \longrightarrow R < R_c \equiv \sqrt{2s_0} l_B$ With small B:

Bound state dissolves if $R_n > \sqrt{2s_0} l_B$.

WKB analysis gives the approximate discrete scale invariance:

$$\ln \frac{R_n}{R_{n-1}} \in \left(\frac{\pi}{s_0} - \frac{1}{2s_0}, \frac{\pi}{s_0} + \frac{1}{2s_0}\right)$$
$$\ln \frac{B_{n+1}}{B_n} \in \left(-\frac{2\pi}{s_0} - \frac{1}{s_0}, -\frac{2\pi}{s_0} + \frac{1}{s_0}\right)$$
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Weyl particle + Coulomb attraction + magnetic field

$$\begin{bmatrix} 0 & \hbar v_F \left(\vec{\sigma} \cdot \vec{k} + \frac{e}{\hbar c} \vec{\sigma} \cdot \vec{A} \right) \\ \hbar v_F \left(\vec{\sigma} \cdot \vec{k} + \frac{e}{\hbar c} \vec{\sigma} \cdot \vec{A} \right) & 0 \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix} = \begin{bmatrix} E - V(R) \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix}$$

Under very large magnetic field with $R_n \gg \frac{\sqrt{2}}{2} Z \alpha l_B$, we consider the lowest landau level solution in cylindrical symmetry (ρ , z, φ).

$$\Psi_{1} = \begin{bmatrix} 0 \\ u(\rho, z)e^{-im\varphi} \end{bmatrix} \quad \Psi_{2} = \begin{bmatrix} 0 \\ v(\rho, z)e^{-im\varphi} \end{bmatrix}$$
$$u(\rho, z) = \rho^{m}e^{-\rho^{2}/4l_{B}^{2}}g(z) \quad v(\rho, z) = i\rho^{m}e^{-\rho^{2}/4l_{B}^{2}}f(z)$$

$$\begin{cases} \frac{E - \tilde{V}(z)}{\hbar v_F} g(z) + \frac{d}{dz} f(z) = 0 \\ \frac{E - \tilde{V}(z)}{\hbar v_F} f(z) - \frac{d}{dz} g(z) = 0 \end{cases} \qquad \tilde{V}(z) = \int_0^\infty \rho^{2m+1} e^{-\rho^2/2l_B^2} \frac{-Z\alpha\hbar v_F}{\sqrt{\rho^2 + z^2}} \frac{d\rho}{m! \, 2^m l_B^{2m+2}} \\ \approx \frac{-Z\alpha\hbar v_F}{z} \left[1 - \frac{(m+1)l_B^2}{z^2} \right] \end{cases}$$

Scale Invariant if $l_B \ll z$ with 1D Coulomb attraction. 22

Weyl particle + Coulomb attraction + magnetic field

$$\left[\frac{d^2}{dz^2} + \frac{d\tilde{V}(z)/dz}{E - \tilde{V}(z)}\frac{d}{dz} + \left(\frac{E - \tilde{V}(z)}{\hbar v_F}\right)^2\right]g(z) = 0$$

$$\left[\frac{d^2}{dz^2} - \frac{3}{4}\left(\frac{\tilde{V}'(z)}{E - \tilde{V}(z)}\right)^2 - \frac{\tilde{V}''(z)}{2\left(E - \tilde{V}(z)\right)} + \left(\frac{E - \tilde{V}(z)}{\hbar v_F}\right)^2\right]\frac{g(z)}{\sqrt{E - \tilde{V}(z)}} = 0$$

For $z \gg l_B$ and $E \approx 0$, attractive potential: $\tilde{V}(z) = -\frac{Z\alpha\hbar v_F}{z}$

$$\left[\frac{d^2}{dz^2} + \frac{(Z\alpha)^2 + 1/4}{z^2}\right]\sqrt{z}g(z) = 0 \quad \Longrightarrow \quad p_z \approx \frac{\hbar Z\alpha}{z}$$

WKB solution:

$$\int_{z_0}^{z_n} p_z \cdot dz = n\pi\hbar \qquad \Longrightarrow \qquad z_n/z_{n-1} = e^{\pi/Z\alpha}$$

Discrete scale invariance 23

Approximate discrete scale invariance

Attractive potential condition:

$$\tilde{V}(z) = \frac{-Z\alpha\hbar v_F}{z} \left[1 - \frac{l_B^2}{z^2} \right] \longrightarrow \frac{l_B}{z_n} < 1$$

Large magnetic field limit

Bound state forms if $z_n > \frac{\sqrt{2}}{2} Z \alpha l_B$.

WKB solution:

$$\int_{z_0}^{z_n} p_z \cdot dz = n\pi\hbar \qquad p_z \approx \frac{\hbar Z\alpha}{z} \left(1 - \frac{l_B^2}{z^2}\right)$$

Approximate discrete scale invariance:

$$\ln \frac{z_n}{z_{n-1}} = \frac{\pi}{Z\alpha} + \frac{2l_{B_n}^2}{z_n^2} - \frac{2l_{B_{n-1}}^2}{z_{n-1}^2} \in \left(\frac{\pi}{Z\alpha} - \frac{4}{(Z\alpha)^2}, \frac{\pi}{Z\alpha} + \frac{4}{(Z\alpha)^2}\right)$$
$$\ln \frac{B_{n+1}}{B_n} \in \left(-\frac{2\pi}{Z\alpha} - \frac{8}{(Z\alpha)^2}, -\frac{2\pi}{Z\alpha} + \frac{8}{(Z\alpha)^2}\right)$$

Comparison to the experimental results

 $v_F \approx 4.5 \times 10^5 \text{ m/s}$ for the Dirac bands in ZrTe₅ [Nature Physics 12, 550 (2016)]

$$Z\alpha \approx 4.87$$
 and $s_0 = \sqrt{(Z\alpha)^2 - 1} \approx 4.77$

Theoretical ratio:

Approximate discrete scale invariance:



Experimental results in ZrTe₅



- 1. Clear demonstration of 5 log-B periodic MR oscillations.
- 2. The experimental scaling factor $\frac{B_n}{B_{n+1}} \in (2,30,4.00)$ is comparable to theoretical estimation.
- The supercritical Coulomb attraction between hole and electron results in two-body Efimov bound states with discrete scale invariance.
- Under magnetic field, the formation and dissolution of Efimov bound states give rise to log-B periodic MR oscillations beyond the quantum limit.

Conclusion

- Coexistence of electron and hole carriers in Weyl system with supercritical Coulomb attraction = twobody Efimov quasi-bound states with discrete scale invariance.
- 2. The formation and dissolution of two-body Efimov quasi-bound states under magnetic field give rise to novel log-B periodic oscillations of 3D systems beyond the quantum limit, where the Landau level physics is inapplicable.

Thank you !

